Hadron spectroscopy and structure from Lattice QCD

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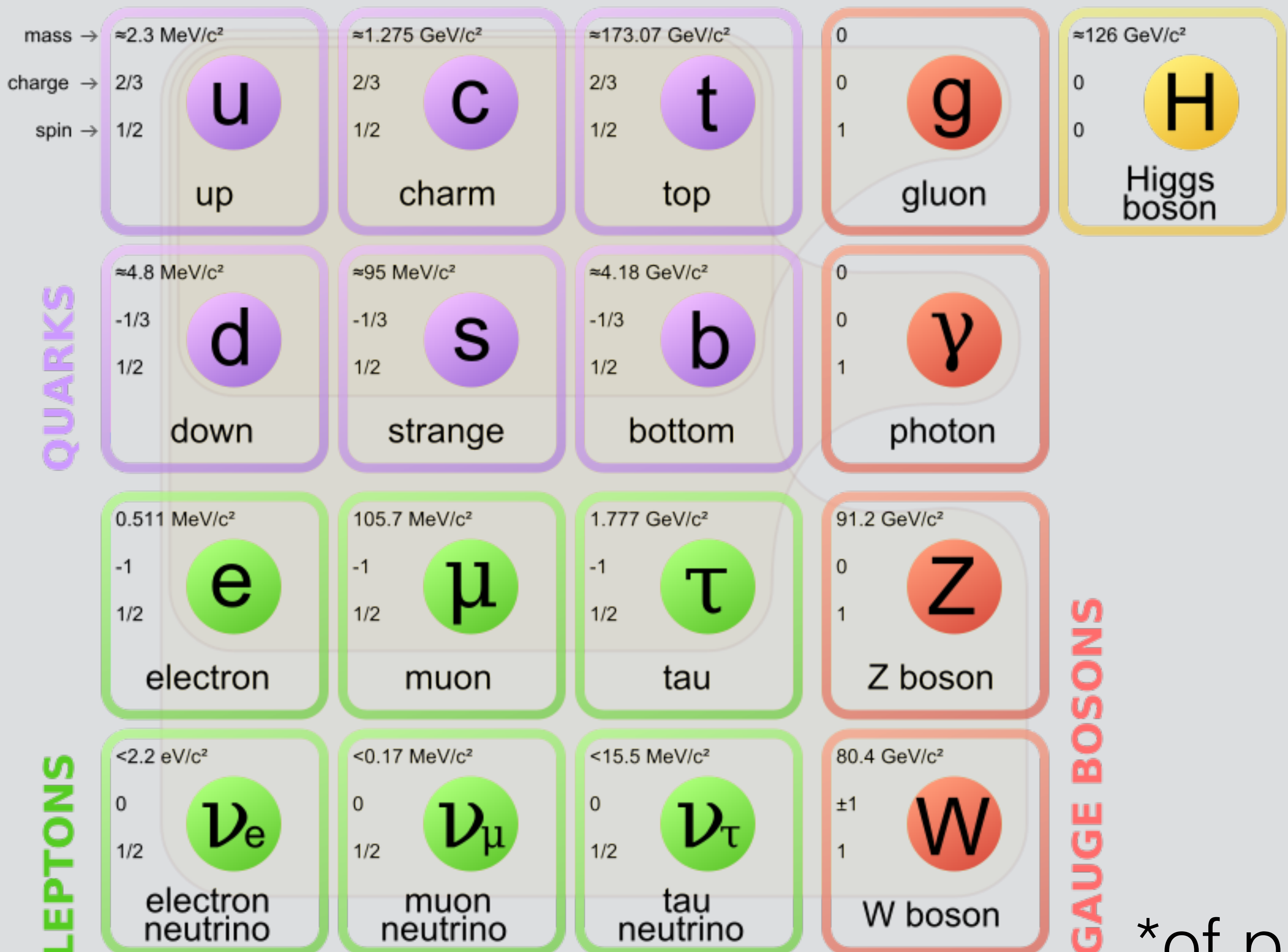
The Standard Model*

Modern picture with 28 free parameters

- gauge couplings (α_s, α_W, α_{QED}), masses (m_l, m_q), CKM and PNMS matrix, EWSB scale



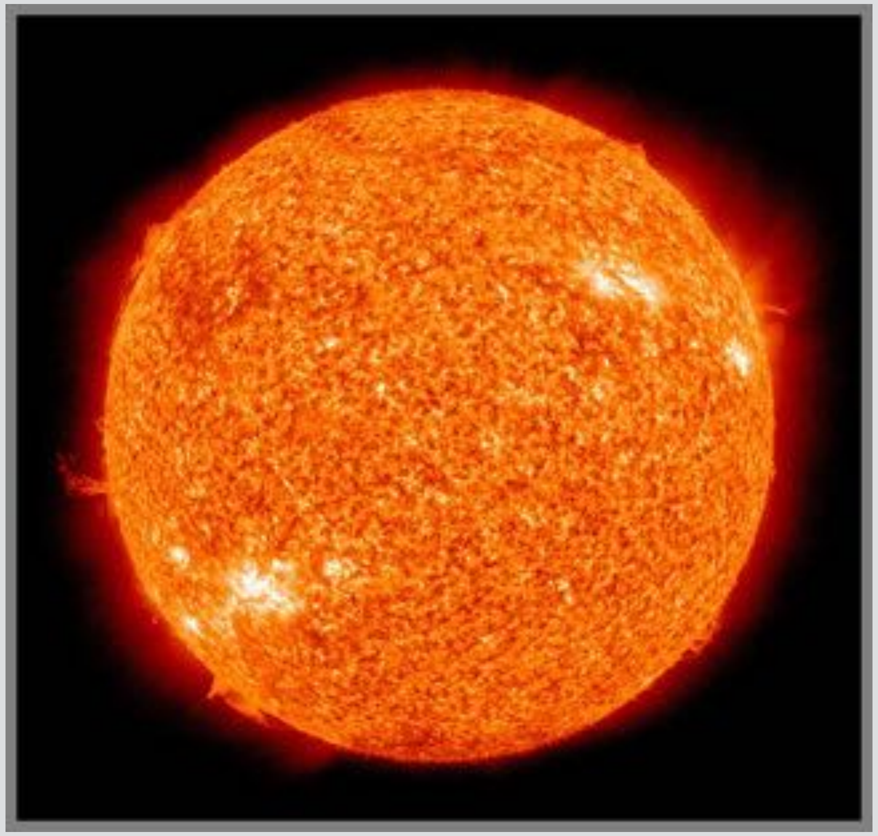
*of particle physics

Quantum Chromodynamics

Theory of the strong interaction
Hadrons governed by QCD (which is most of our world!)

How our sun works!

$$p + p \to d + e^+ + \nu_e$$



Particle decay

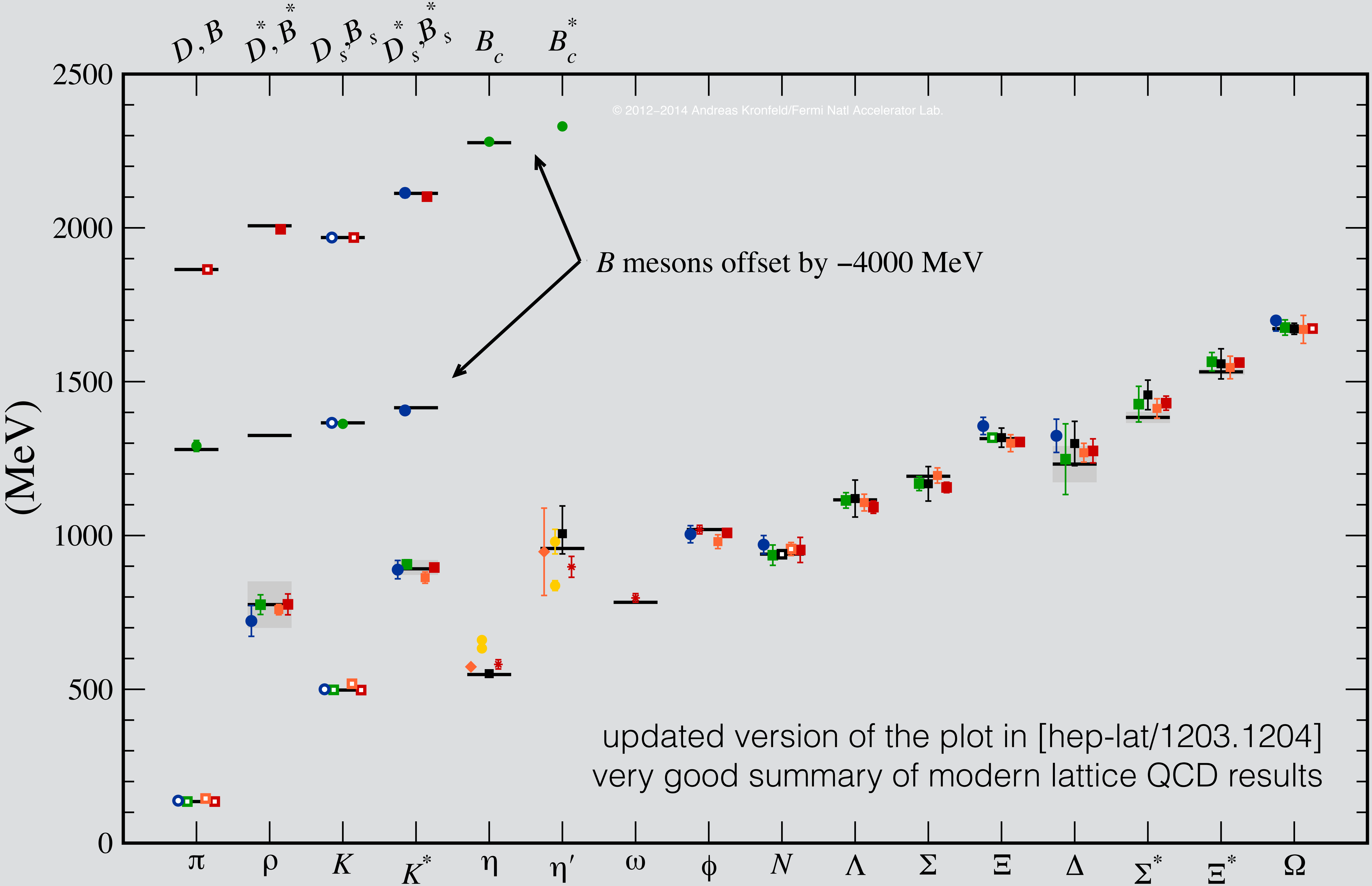
$$B \to \pi + \ell + \nu$$

Neutral meson oscillations

$$K \to \bar{K}$$

Experiments involving hadrons need theoretical input from QCD at typical hadronic energy which is *non-perturbative*

Lattice QCD spectroscopy



Outline

Generating data from a QCD simulation

- How to construct a hadron (spectroscopy)
- How to describe hadrons interactions (structure)

What did we actually simulate?! (it’s messy)

- Spectral decomposition of correlation functions

How do we get physics from all this mess!

- A sample of some data analysis techniques

QCD vacuum on the computer

Numerically tackle QCD from Path Integral formulation

For any observable *A*

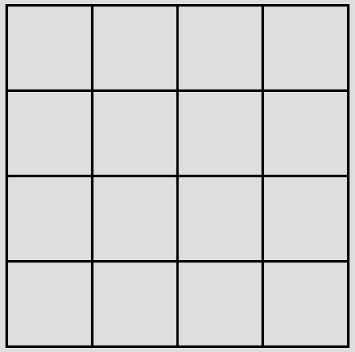
$$\langle A \rangle = \frac{1}{Z} \int [d\psi][d\bar{\psi}][dU] A[\psi, \bar{\psi}, U] e^{-S_U - S_D}$$

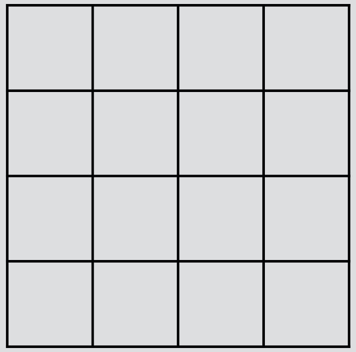
Wick-rotate to imaginary time
(integral becomes local so it fits on a computer)

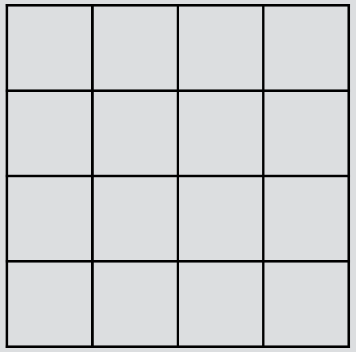
(Very) High-dimensional integral (x, y, z, t, spin, color)
Monte Carlo integration only affordable method

$$U \sim e^{-S_U + \ln \det(\not{D} + m)}$$

(importance sampling)







Life on the Lattice*

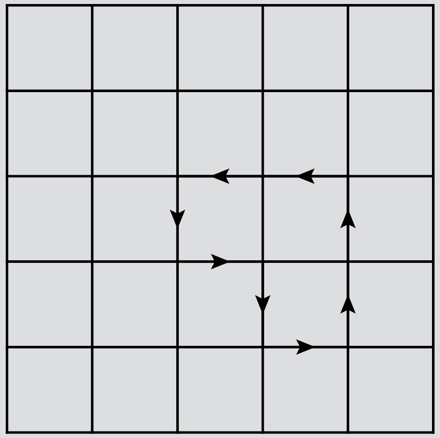
*fun lattice blog to read
http://latticeqcd.blogspot.com/

weighted average is now a simple average

$$\langle \Omega | A | \Omega \rangle \simeq \frac{1}{N} \sum_{n=1}^{N} A(U_n) \quad \text{where} \quad U \sim e^{-S_U + \ln \det(\not{D} + m)}$$

reuse gauge configurations for different *A*
(otherwise calculations will be unaffordable)

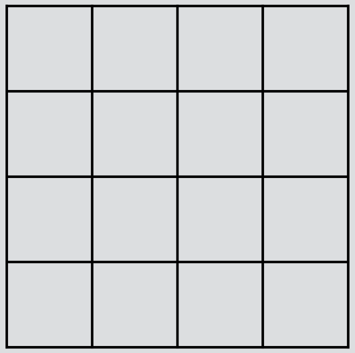
at 1 cent / cpu hour (electric bill) the U's cost millions of dollars



- valence quarks live on lattice sites
- sites are connected by links (gauge fields, parallel transport operators)
- observables are closed loops (gauge invar.)

[hep-lat/0506036] (very good introductory paper to lattice QCD)

Making hadrons on the lattice



Have many observations of the QCD vacuum
Now make a hadron!

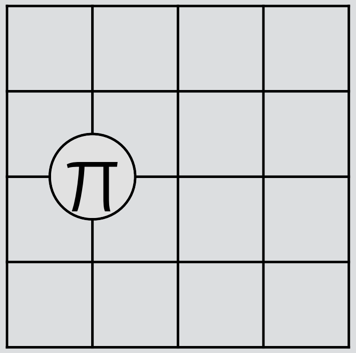
What is a ground state pion? (look at PDG)

- two valence light quarks (isospin symmetric limit)
- spin zero
- angular momentum zero (s-wave)
- radial excitation zero
- negative parity

$$J^P = 0^-$$

Guess the creation operator!

$$\pi \equiv \bar{q}_i^a \gamma_5^{ij} q_j^a$$



spherical symm.
pseudoscalar
no spin

Making correlation functions

Two-point correlation function

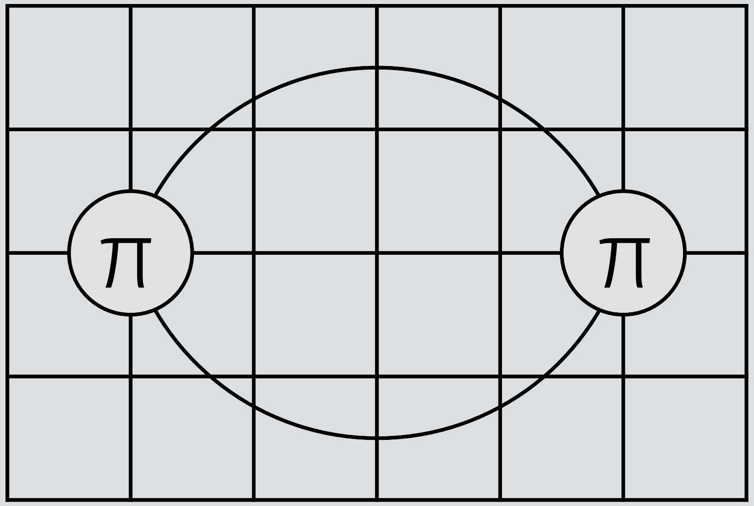
$$C^{2pt}(x,0) = \langle T\{\bar{q}_i^a(x)\gamma_5^{ij} q_j^a(x)\bar{q}_k^b(0)\gamma_5^{kl} q_l^b(0)\}\rangle$$

Rewrite as quark propagators $L_{ij}^{ab}(x,0) = q_i^a(x)\bar{q}_j^b(0)$

$$\begin{aligned} C^{2pt}(x,0) &= -\, L_{li}^{ba}(0,x)\gamma_5^{ij} L_{jk}^{ab}(x,0)\gamma_5^{kl} \\ &= -\, \mathrm{Tr}_{c,D}\{L^\dagger(x,0)L(x,0)\} \end{aligned}$$

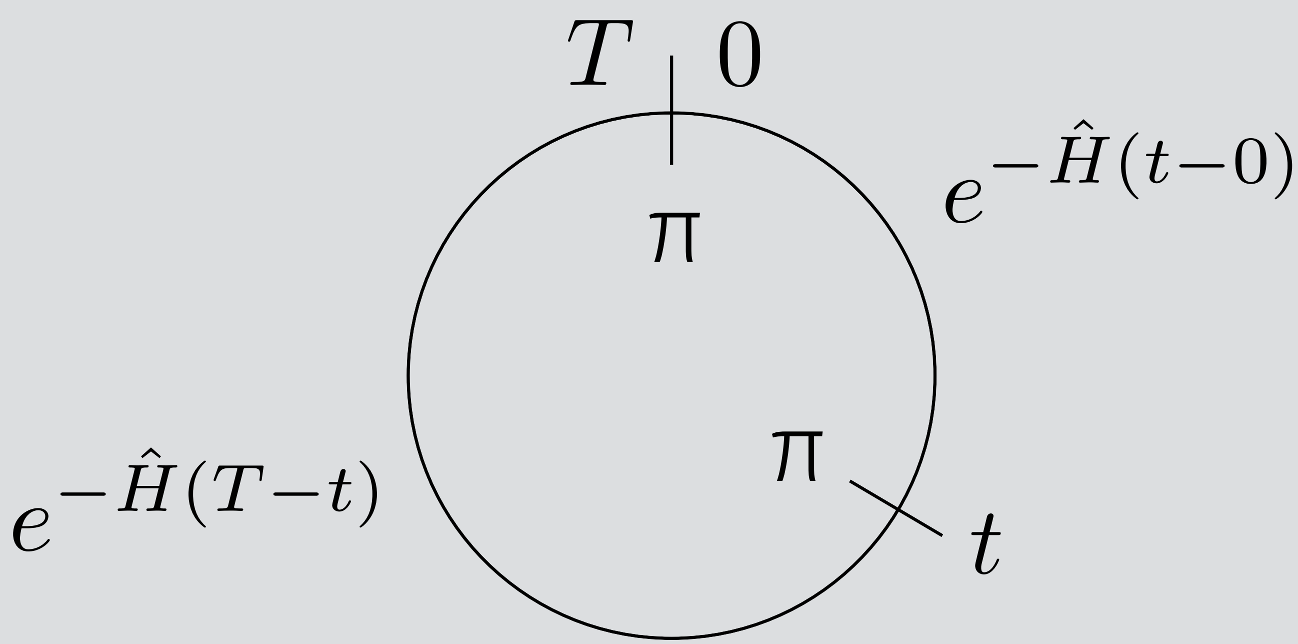
Propagator is inverse of Dirac operator (a matrix)

This is how a correlation function is calculated!



Spectral decomposition

We calculated a pion + junk
How do we get the pion out of this?



resolution of the identity

$$1 = \sum_n \frac{|n\rangle\langle n|}{2E_n}$$

the pion creation operator couples to radial excitations

$$C^{2pt}(t) = \sum_{n,m} \frac{1}{4E_n E_m} \langle n|\bar{\pi} e^{-\hat{H}(t)}|m\rangle\langle m|\pi e^{-\hat{H}(T-t)}|n\rangle$$

Spectral decomposition

Project out energy eigenstates

Assume zero temperature (Large box size in time)

$$C^{2pt}(t) = \sum_{n,m} \frac{1}{4E_n E_m} \langle n|\bar{\pi} e^{-\hat{H}(t)}|m\rangle\langle m|\pi e^{-\hat{H}(T-t)}|n\rangle$$

$$= \sum_{n,m} \frac{e^{-E_m t} e^{-E_n (T-t)}}{4E_n E_m} \langle n|\bar{\pi}|m\rangle\langle m|\pi|n\rangle$$

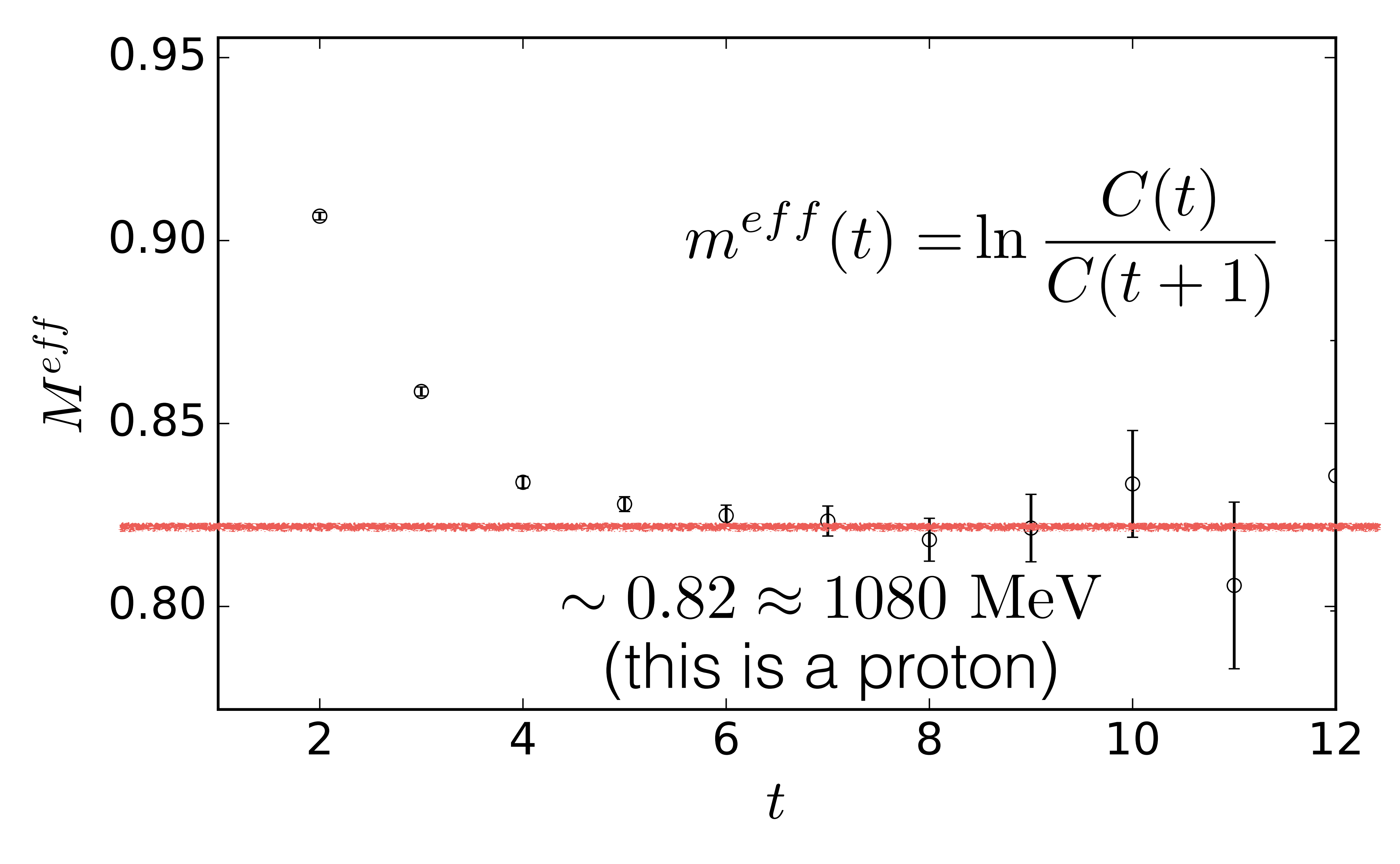
$$\simeq \sum_{n} \left[\frac{e^{-E_n t}}{2E_n} \langle \Omega|\bar{\pi}|n\rangle\langle n|\pi|\Omega\rangle + \frac{e^{-E_n (T-t)}}{2E_n} \langle \Omega|\pi|n\rangle\langle n|\bar{\pi}|\Omega\rangle \right]$$

We have an infinite sum of exponentials…

Getting the pion mass

We have 1) data 2) spectral decomposition

$$C^{2pt}(t) = -\sum_{\vec{x}} \mathrm{Tr}_{c,D}\{L^\dagger L\} \qquad C^{2pt}(t) \simeq \sum_n \frac{Z_n^2}{2E_n} e^{-E_n t}$$



Data distribution

We want the distribution of the **mean**

central limit theorem promises multivariate normal

$$P(C_t|Z,E) = \frac{1}{\sqrt{(2\pi)^{\nu}|\Sigma|}} e^{-\frac{1}{2}(y-\mu)_{t_1}\Sigma^{-1}_{t_1,t_2}(y-\mu)_{t_2}}$$

$$\propto e^{-\chi^2_{\mathrm{data}}/2}$$

where Σ is the standard error of the mean squared

$$\Sigma_{t_1,t_2} = \frac{1}{N}\left[\frac{1}{N}\sum_{i,j}^{N}(C_i-\mu)_{t_1}(C_j-\mu)_{t_2}\right]$$

Getting mass the frequentist way

Perform a maximum likelihood estimate of parameters

Likelihood = Probability of finding data given parameters

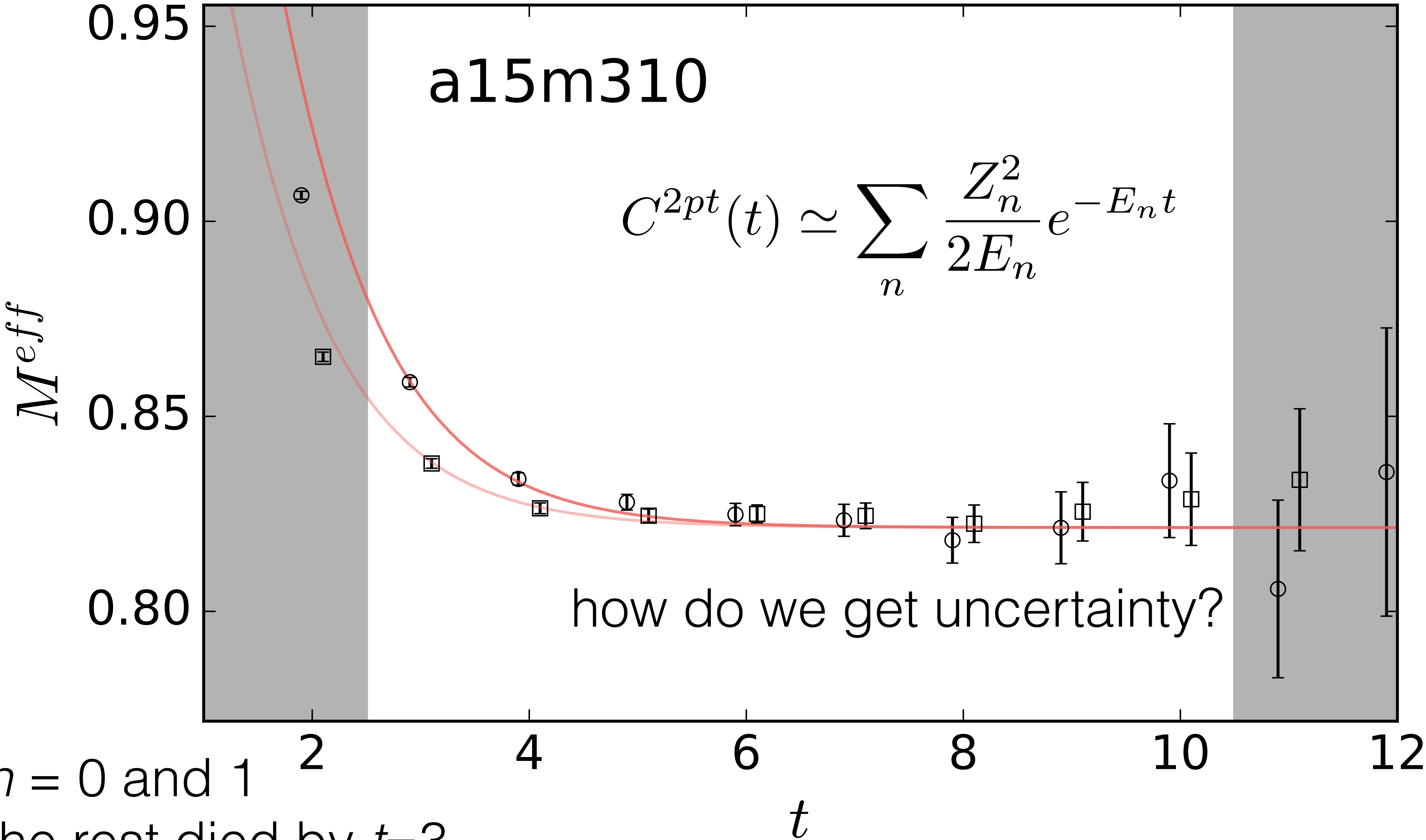
$$L \sim e^{-\frac{1}{2}[C^{2pt}(t)-\overline{\mathrm{data}}(t)]^T \Sigma^{-1} [C^{2pt}(t)-\overline{\mathrm{data}}(t)]}$$

Minimize the χ^2 to get best fit to data

Take data and try to fit with (truncate the sum)

$$C^{2pt}(t) \simeq \sum_n \frac{Z_n^2}{2E_n} e^{-E_n t}$$

Getting mass the frequentist way



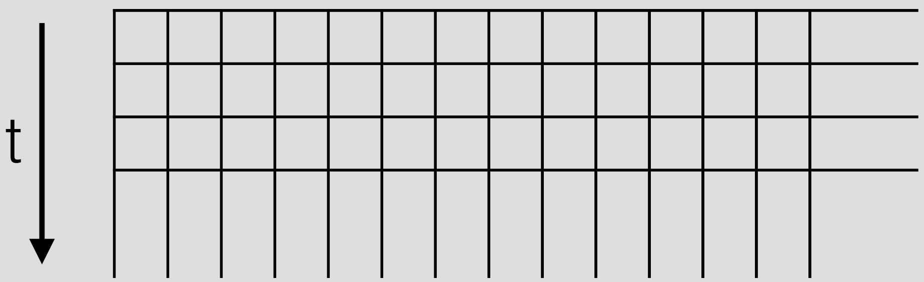
n = 0 and 1
the rest died by t=3

Frequentist error estimation

Bootstrap resampling

1 2 3 4 5 6 7 … (config.)

original data t

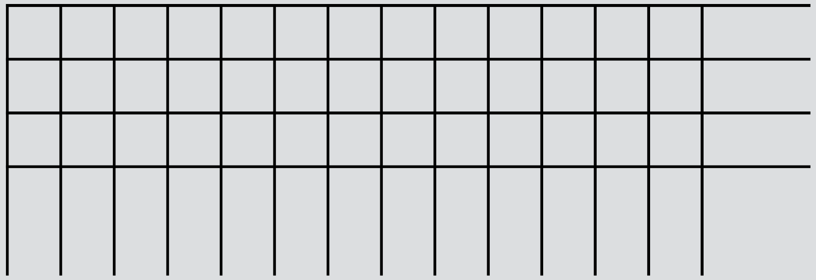


boot0

fit this data get results for fit parameters (masses, etc)

draw with replacement

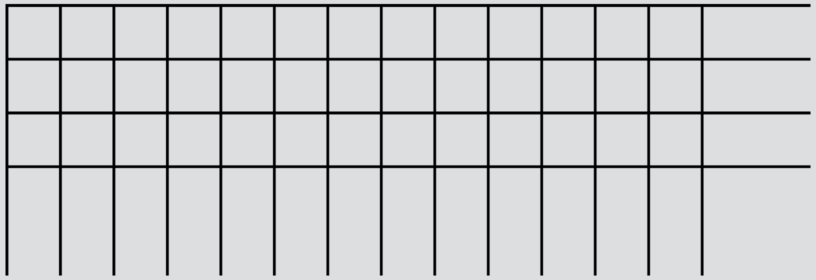
4 7 7 8 2 1 9 1 2 …



bootstrap resample 1

fit data get result

5 7 8 8 2 1 9 8 3 …



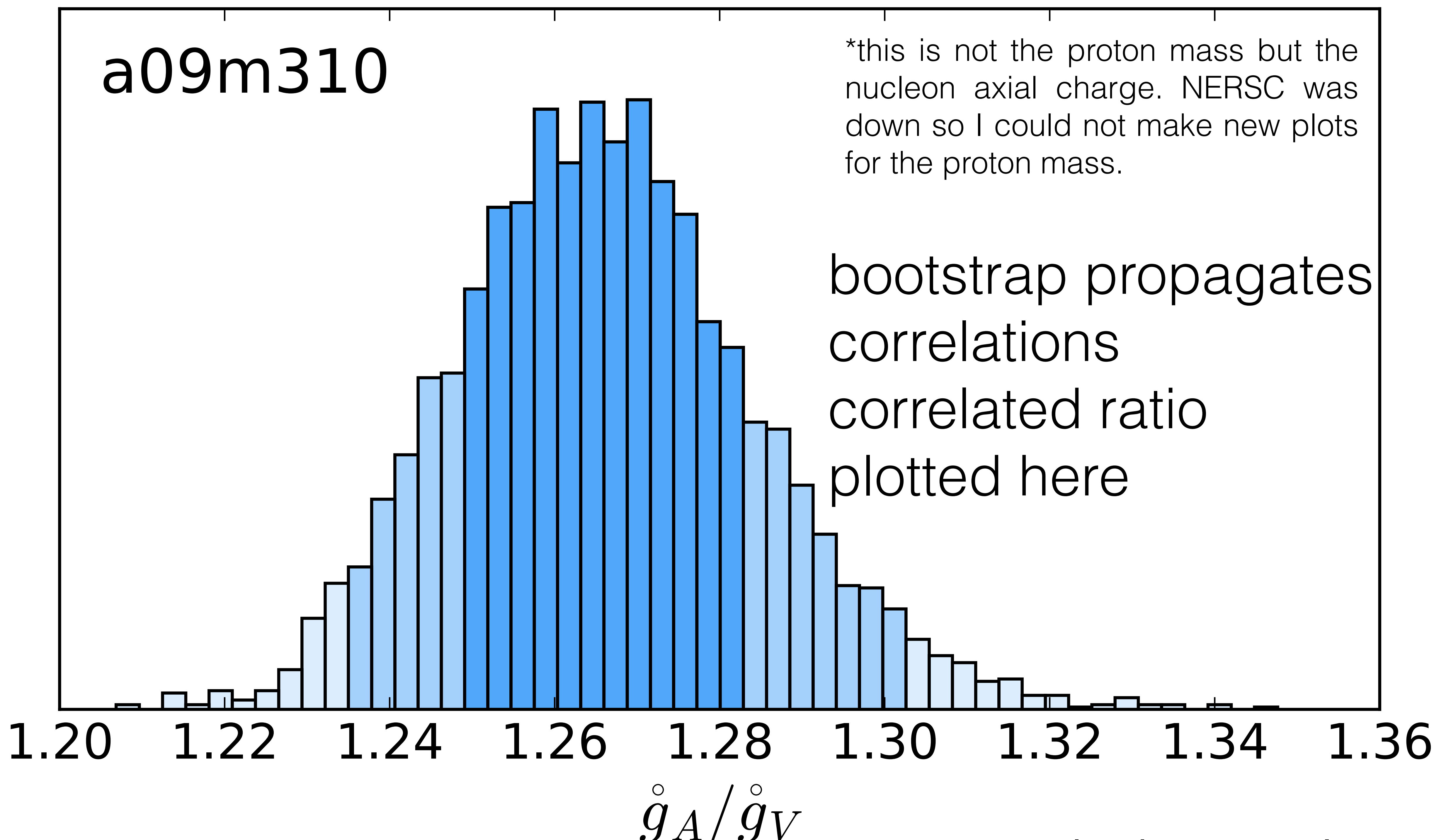
bootstrap resample 2

fit data get result

… repeat

Bootstrap histograms

Result of the bootstrap resampling on a fit parameter

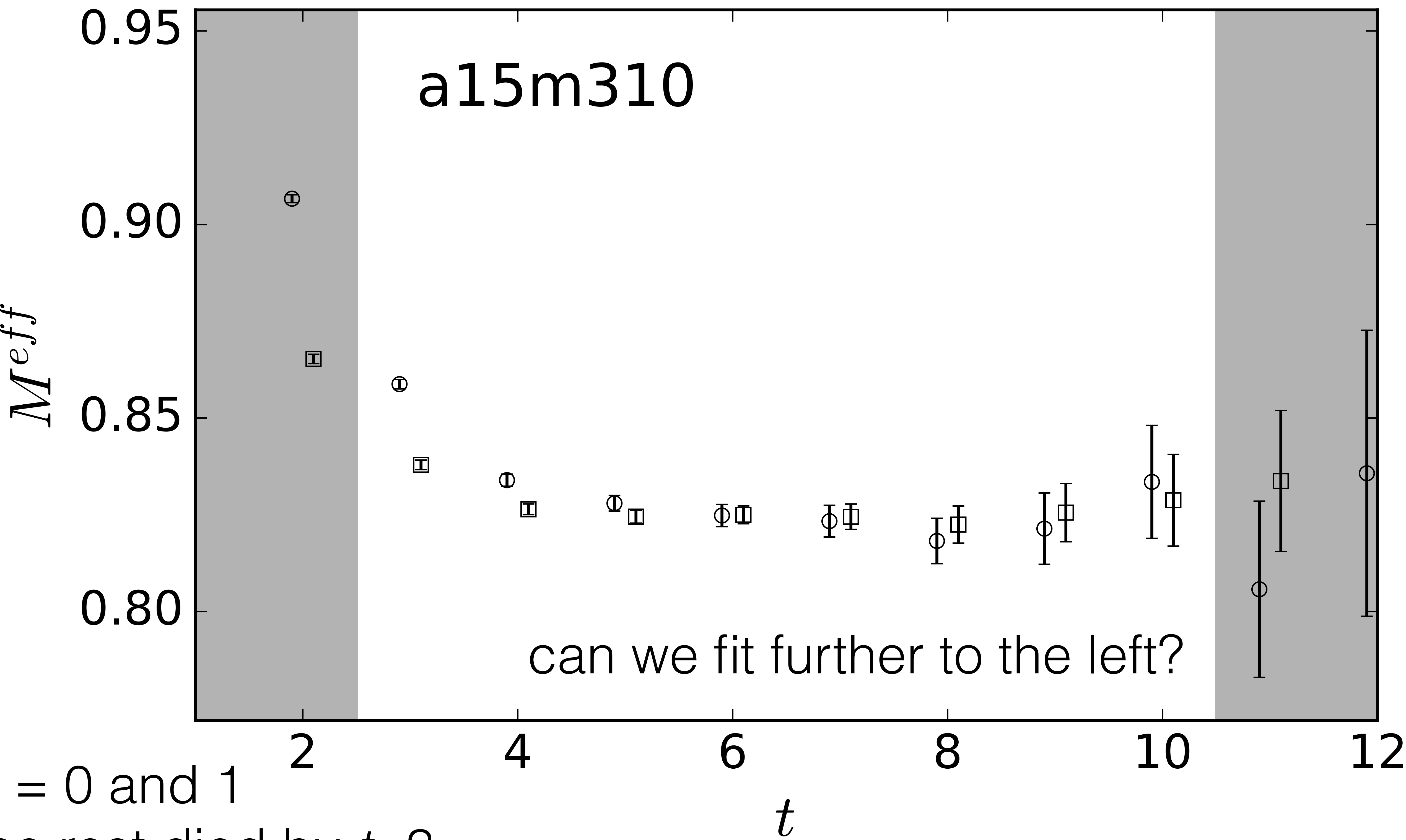


*this is not the proton mass but the nucleon axial charge. NERSC was down so I could not make new plots for the proton mass.

bootstrap propagates correlations
correlated ratio plotted here

resampled 4000 times

Reconstruct fit with bootstrap



n = 0 and 1
the rest died by t=3

Bayesian constraint curve fit

sum of exponentials is ill-conditioned
motivate constraint via Bayes theorem

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

mean distribution of fit parameters are normal also

$$P(Z,E) \propto e^{-\chi^2_{\mathrm{prior}}/2}$$

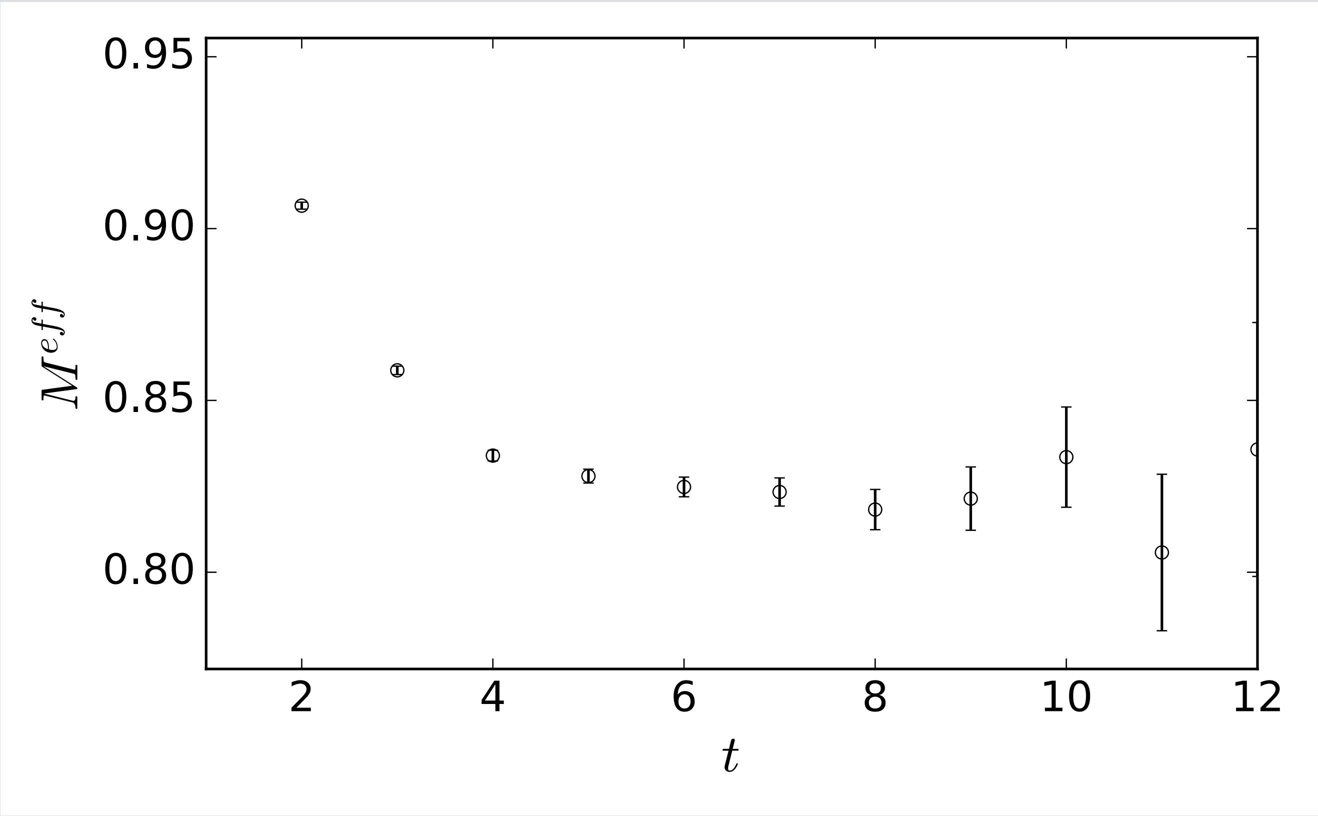
- we have approximate conjugate priors
- normalization factor is trivial

we do not need MC to obtain the posterior distribution

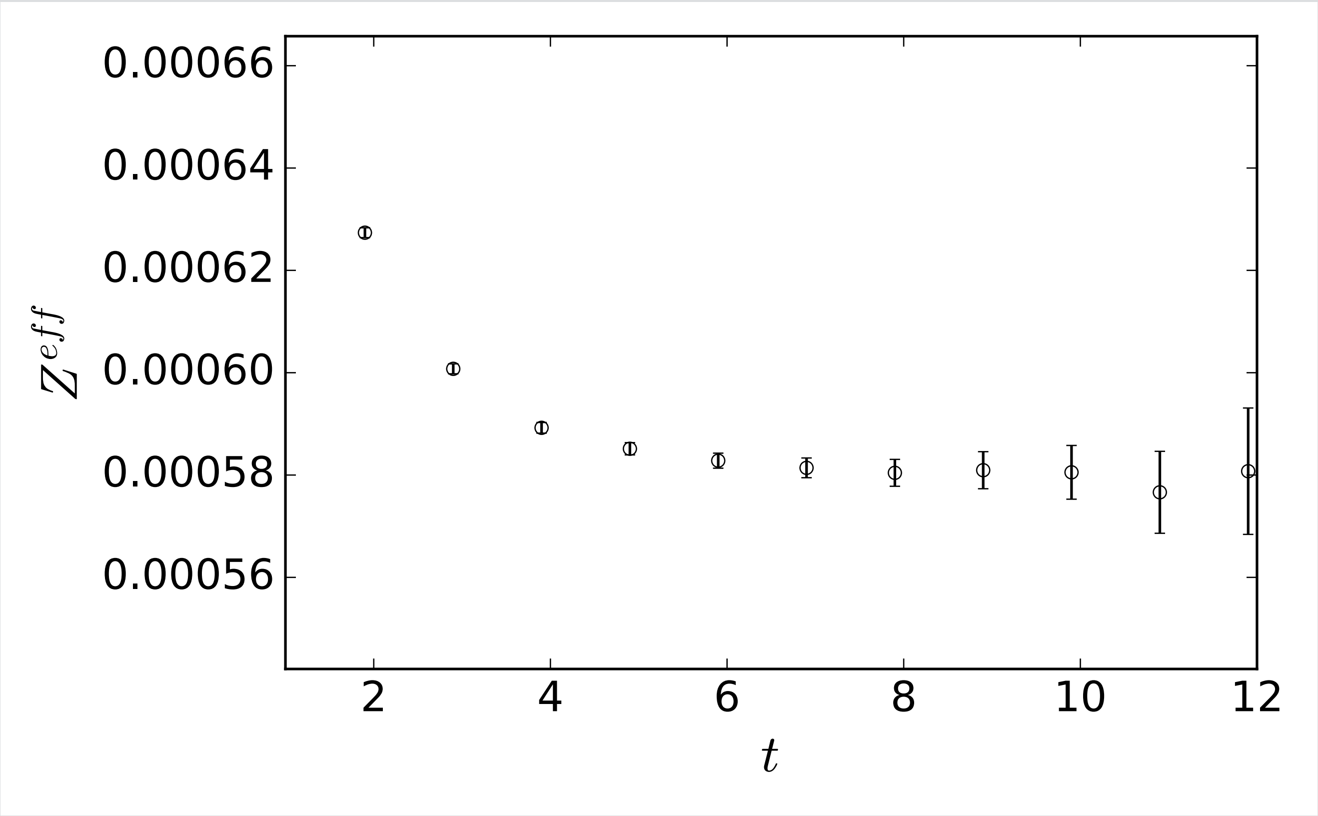
$$P(Z,E|C_t) \propto e^{-(\chi^2_{\mathrm{data}}+\chi^2_{\mathrm{prior}})/2}$$

Prior constraints

Ground state energy



Ground state overlap

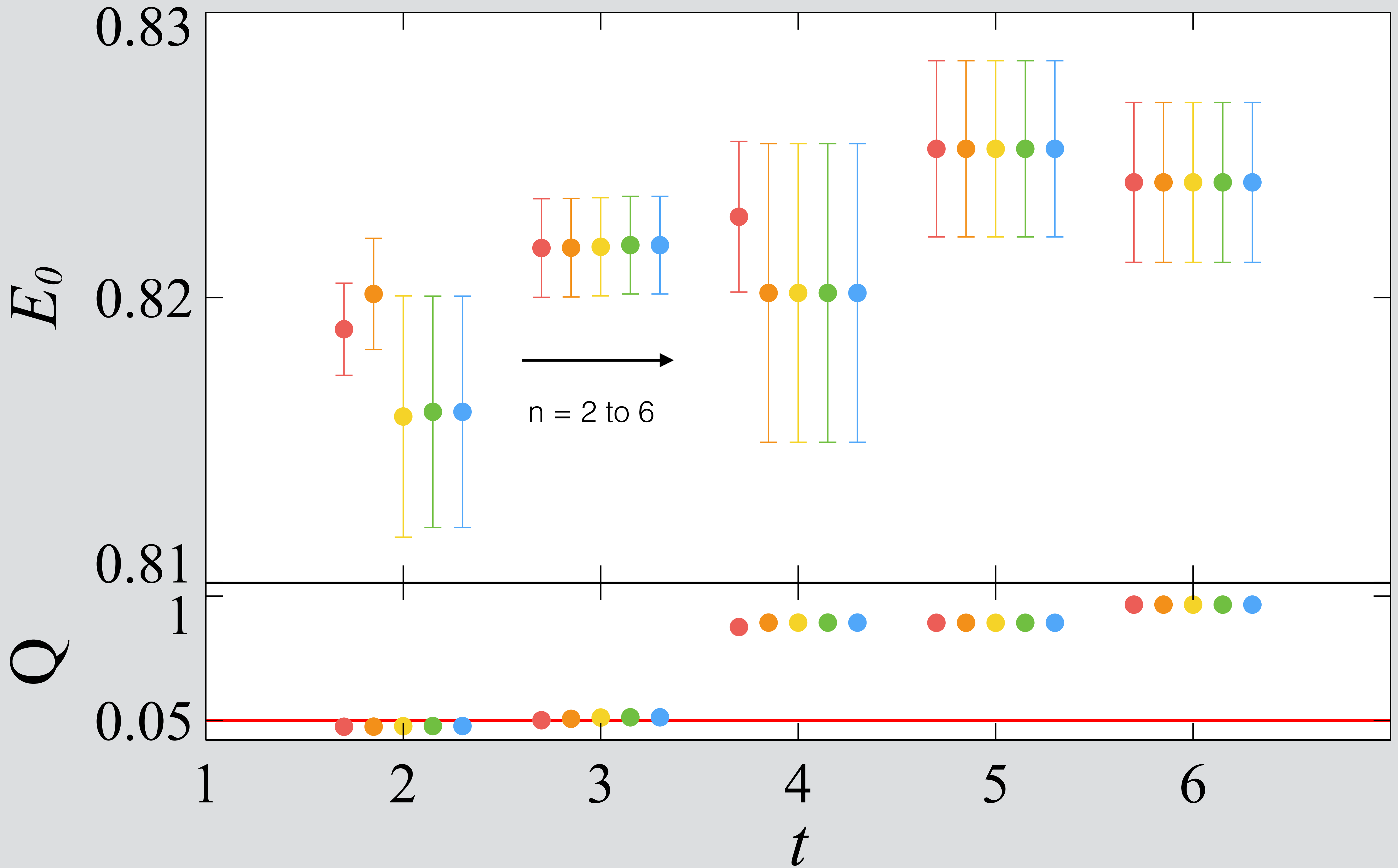


Excited state energy ~ Roper resonance

Excited state overlap ~ same order of magnitude

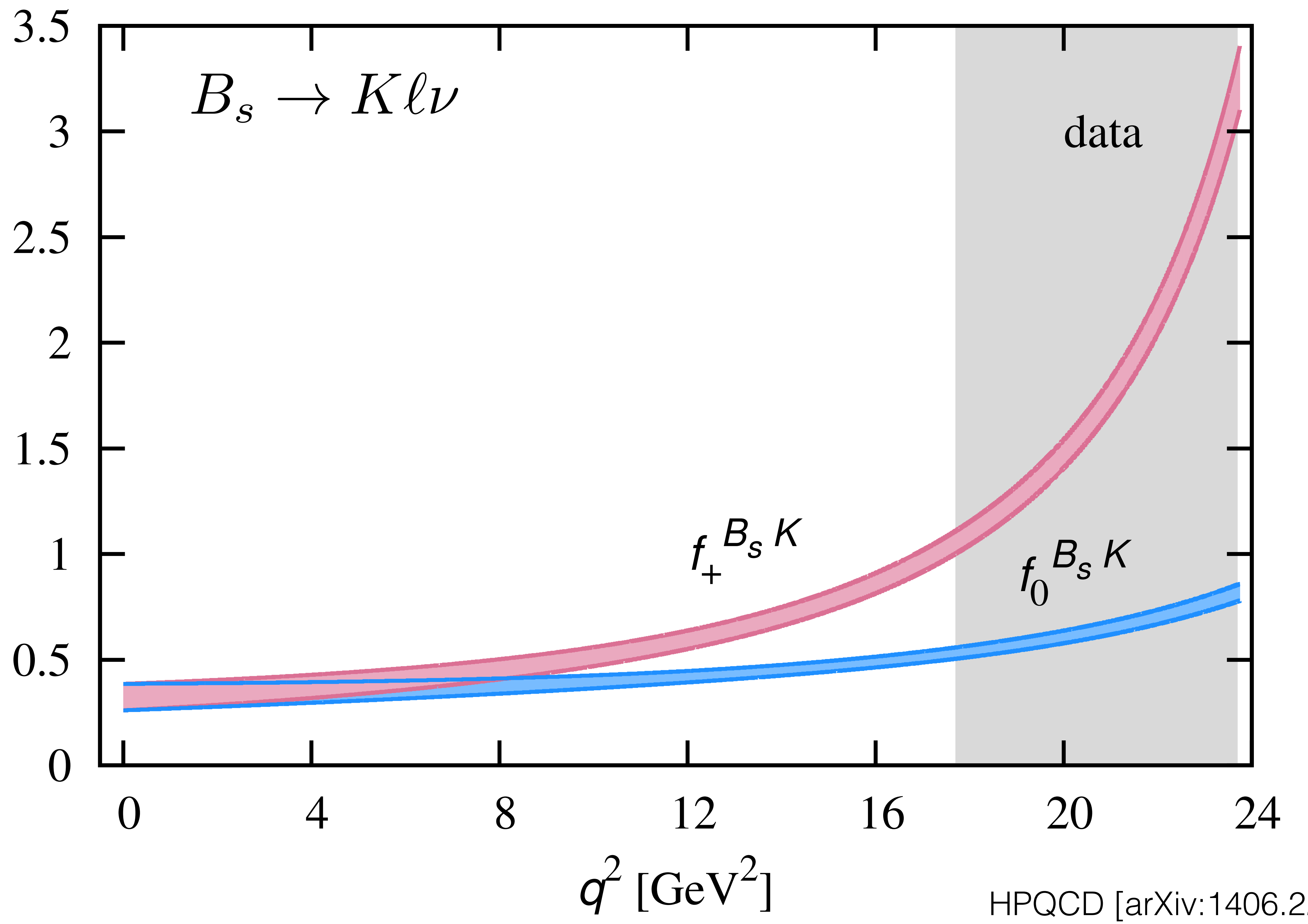
Stability plot

Ok… for this dataset t=3 is the best we can do…



Structure calculations

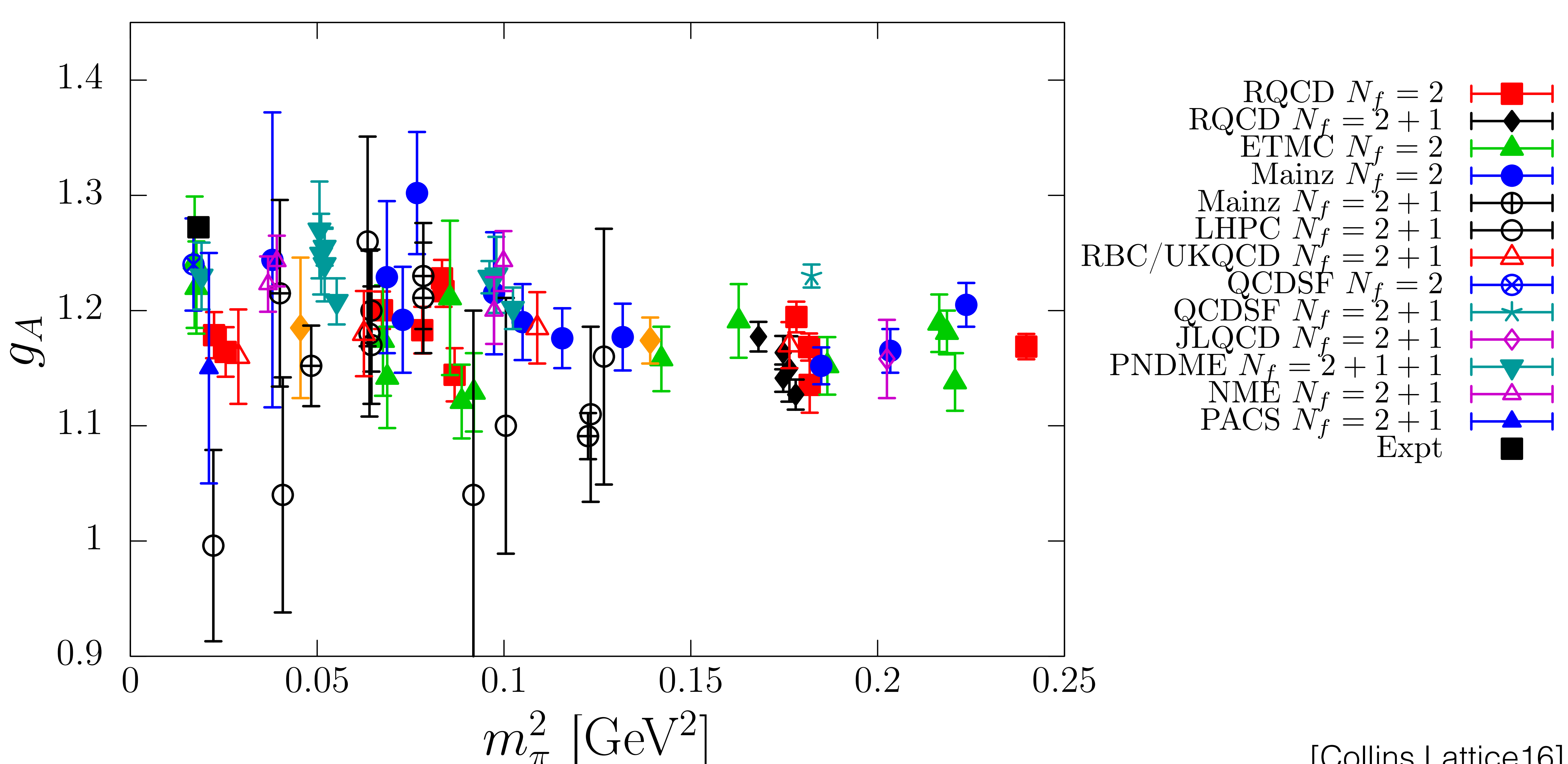
Understand how hadrons interact with other particles



HPQCD [arXiv:1406.2279]

Nucleon axial charge

Benchmark calculation of lattice QCD for nuclear physics



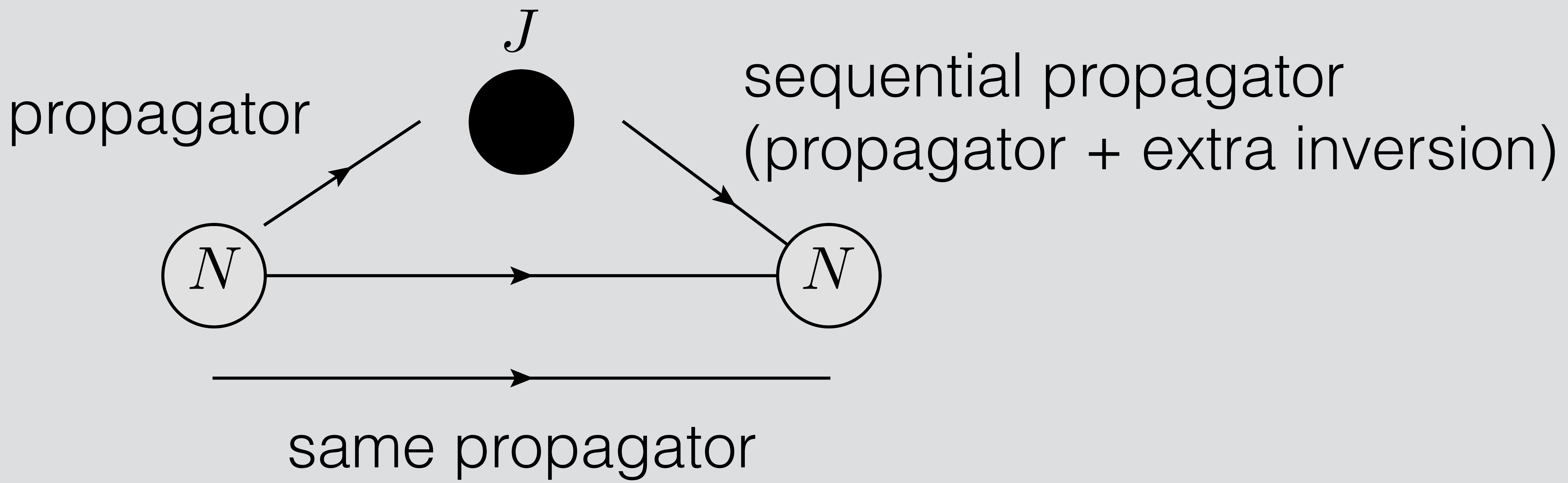
[Collins Lattice16]

Simplest structure calculation for baryons

Lattice calculations systematically low (problem!)

Three-point correlation functions

Insert axial-vector current between nucleons

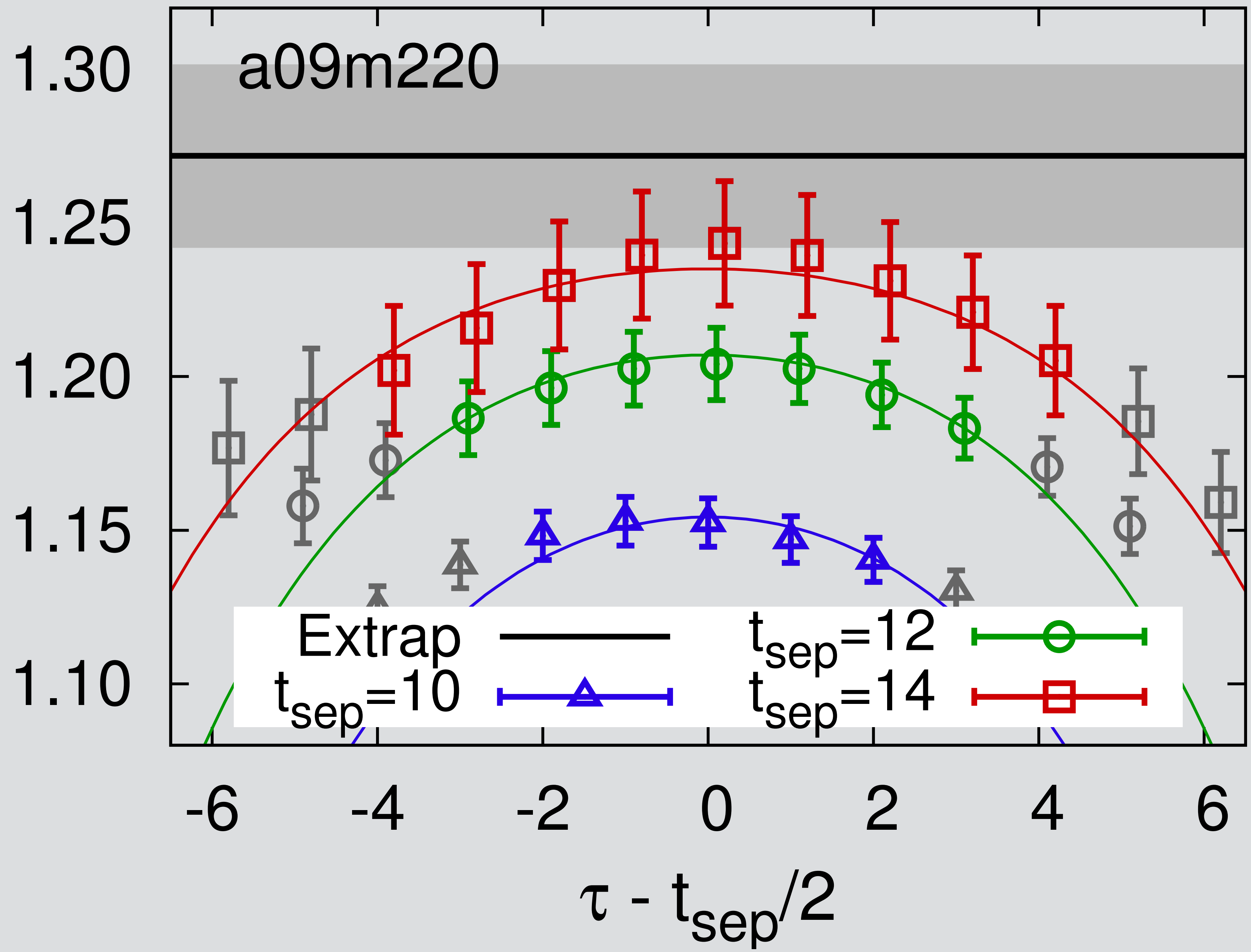


sequential propagators invert off hadronic sink
source-sink separation has to be fixed as a result
can insert any current once propagators are created

PNDME nucleon axial current

[1606.07049]

At fixed t_{sep} excited state contamination is sum of constants



x-axis is current insertion time

excited states disappear at large t_{sep} where large is not large enough

signal degrades exponentially

better data generation?
better analysis?

Feynman-Hellmann Theorem

Matrix elements are related to variations in the spectrum with respect to an external source

$$\frac{\partial E_n}{\partial \lambda} = \langle n|H|n\rangle$$

where

$$S = S_{\mathrm{QCD}} + S_\lambda$$

The external source is

$$S_\lambda = \lambda \int d^4 x j(x)$$

of some bilinear current density (*e.g.* axial-vector current)

An interesting new way to calculate nucleon structure

[1612.06963] Awesome paper (I'm an author)

FHT on the lattice

Reminder: Effective mass

$$m^{eff}(t) = \ln \frac{C(t)}{C(t+1)}$$

Take the analytic derivative w.r.t. external source

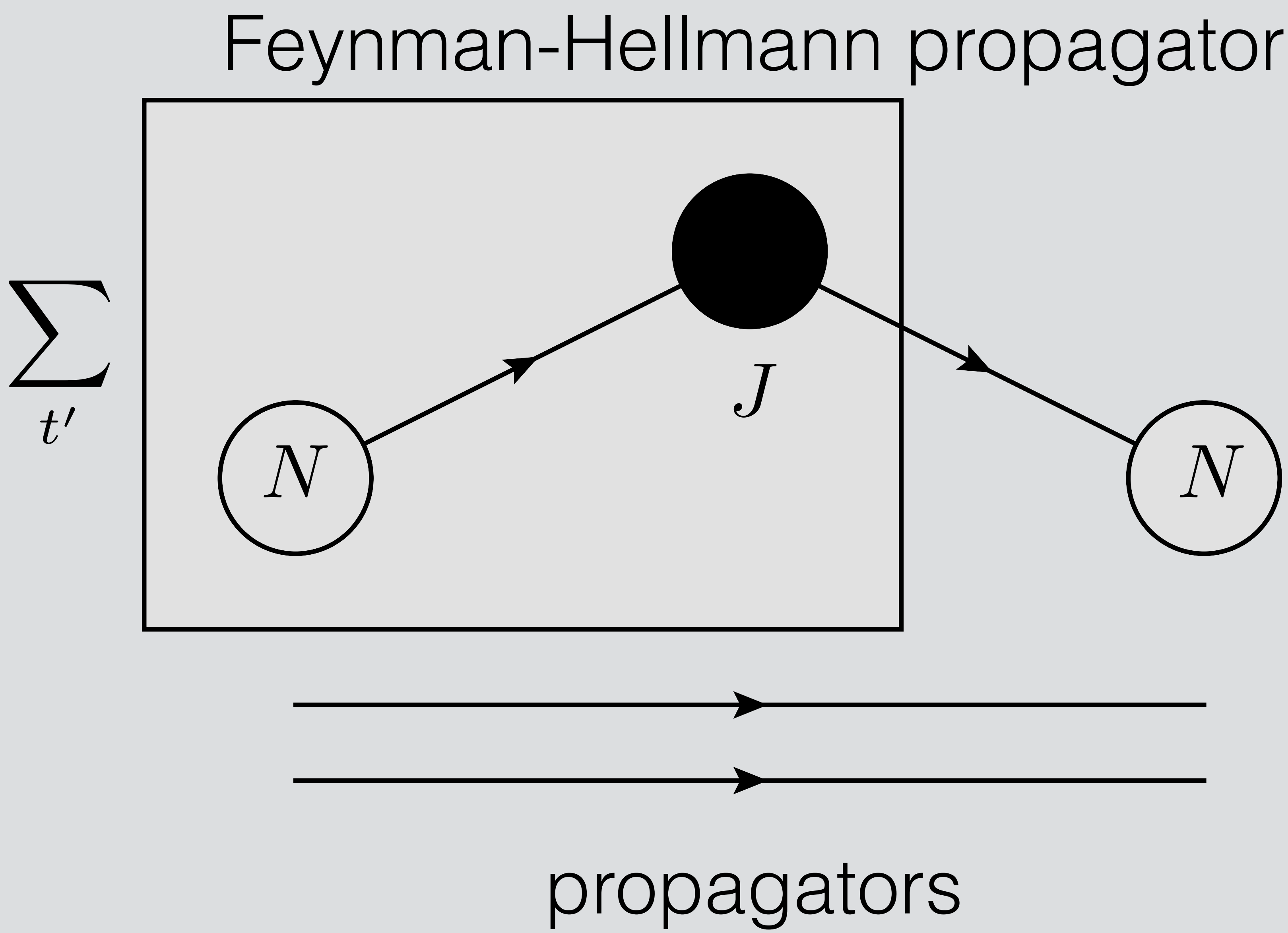
$$\left.\frac{\partial m^{eff}}{\partial \lambda}\right|_{\lambda=0} = \left.\left[\frac{\partial_\lambda C_\lambda(t+1)}{C_\lambda(t+1)} - \frac{\partial_\lambda C_\lambda(t)}{C_\lambda(t)}\right]\right|_{\lambda=0}$$

where

$$-\partial_\lambda C_\lambda(t)|_{\lambda=0} = -\, C(t) \int dt' \langle \Omega | J(t') | \Omega \rangle$$
$$+ \int dt' \langle \Omega | T\{N(t) J(t') N^\dagger(0)\} | \Omega \rangle$$

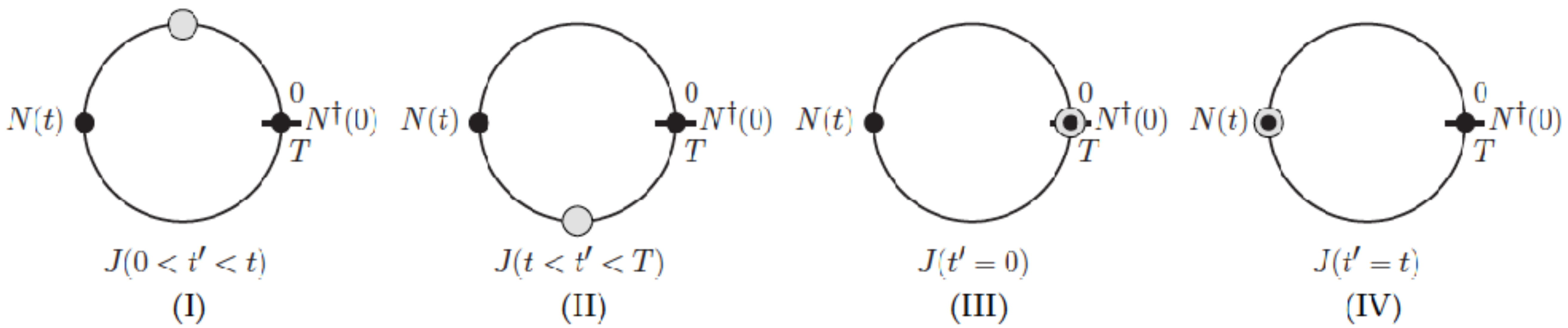
First term vanishes unless it is a scalar current
Second term is sequential propagator through the current

Feynman-Hellmann propagator



Current is point-like so sum over time (and space) is valid
Generate data as a function of source-sink separation

Spectral decomposition



signal artifacts from summing over all current time

Go to Heisenberg picture and insert identity…

$$\partial_\lambda C_\lambda(t)|_{\lambda=0} = \sum_n \left[(t-1) z_n g_{nn} z_n^\dagger + d_n\right] e^{-E_n t}$$

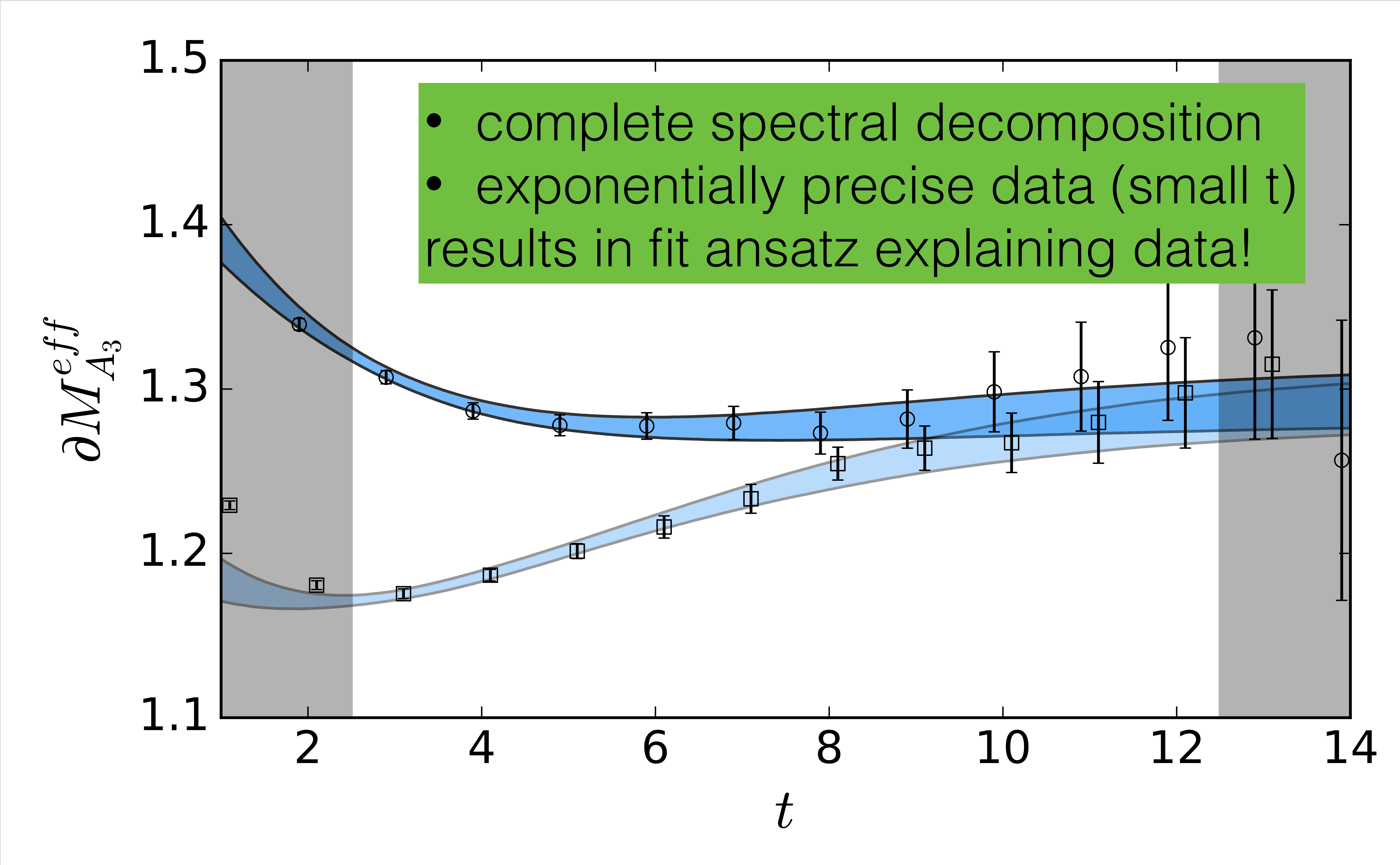
$$+ \sum_{n \neq m} z_n g_{nm} z_m^\dagger \frac{e^{-E_n t} e^{\Delta_{nm}/2} - e^{-E_m t} e^{\Delta_{mn}/2}}{e^{\Delta_{mn}/2} - e^{\Delta_{nm}/2}}$$

luckily all the artifacts can be absorbed into d_n

still the spectral decomposition is quite daunting

Feynman-Hellmann fits

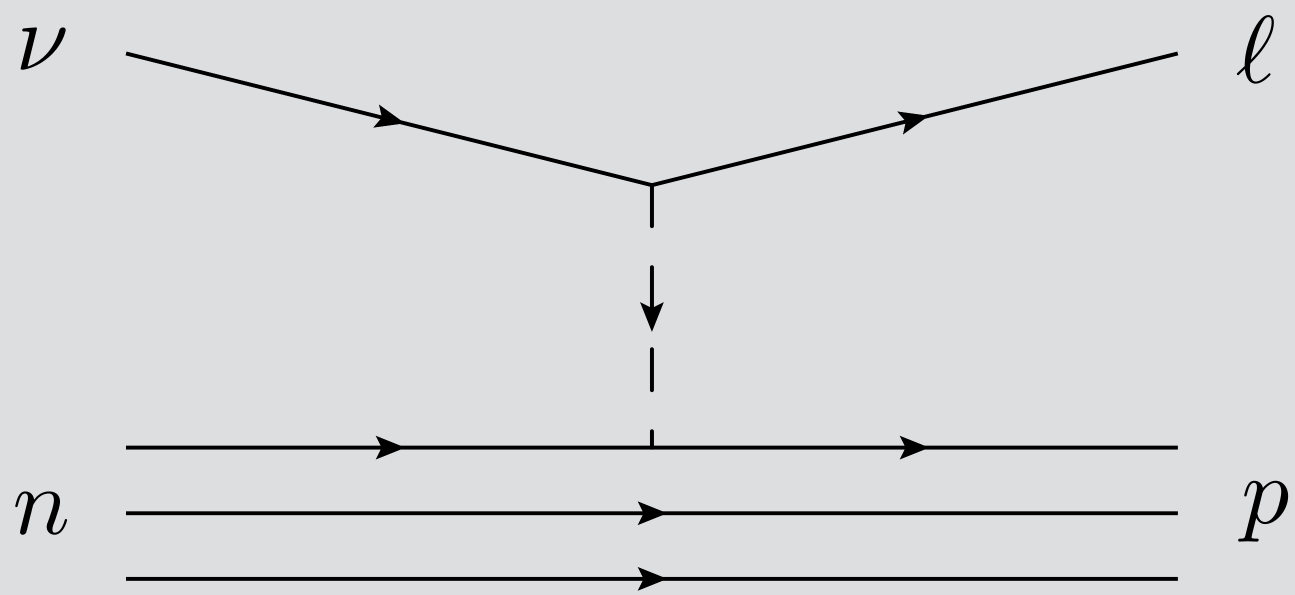
Just be brave



ν-N quasi-elastic scattering

Llwewllyn-Smit formalism

$$\frac{d\sigma}{dQ^2}\begin{pmatrix}\nu n \to \ell^- p \\ \overline{\nu} p \to \ell^+ n\end{pmatrix} = \frac{M_N^2 G_F^2 |V_{ud}|^2}{8\pi E_\nu^2} \times \left[A(Q^2) \mp B(Q^2)\frac{s-u}{M_N^2} + \frac{C(Q^2)(s-u)^2}{M_N^4}\right]$$



form factors

$$\sim F_1(Q^2), F_2(Q^2), F_A(Q^2)$$

$$F_A(Q^2) = g_A\left(1+\frac{Q^2}{M_A^2}\right)^{-2}$$

~1% uncertainty for g_A before isospin & EM effects dominate

Llwewllyn-Smit [Phys.Rept. 3 (1972) 261-379]

Proton charge radius

Gordon decomposition of vector current

$$\langle 0|V_4|q_3\rangle = \overline{u}(0)\left(\gamma_4 F_1(Q^2) + \frac{i}{2M_N}\sigma_{43}q^3 F_1(Q^2)\right)u(q_3)$$
$$= 2E_N F_1(Q^2)$$

calculate slope of F_1 on the lattice

$$\left.\frac{\partial G_E(Q^2)}{\partial Q^2}\right|_{Q^2=0} = -\frac{1}{6}\langle r^2\rangle = \left.\frac{\partial F_1(Q^2)}{\partial Q^2}\right|_{Q^2=0} - \frac{F_2(0)}{4M_N^2}$$

7σ experimental *e vs. μ* discrepancy
~2% uncertainty can discriminate 4% exp. difference

lattice can provide model independent values for radii

Carlson [arXiv:1502.05314v1]

Moment methods

Relate spatial moments to momentum derivatives

Issues with moment methods:

Wilcox - Moments on lattice yields wrong ground state.

[0204024v1]

Existing methods:

Isgur-Wise slope - position space method [9410013]

HVP - time moment current current correlator [1403.1778v2]

Rome - expand lattice operators [1208.5914v2][1407.4059]

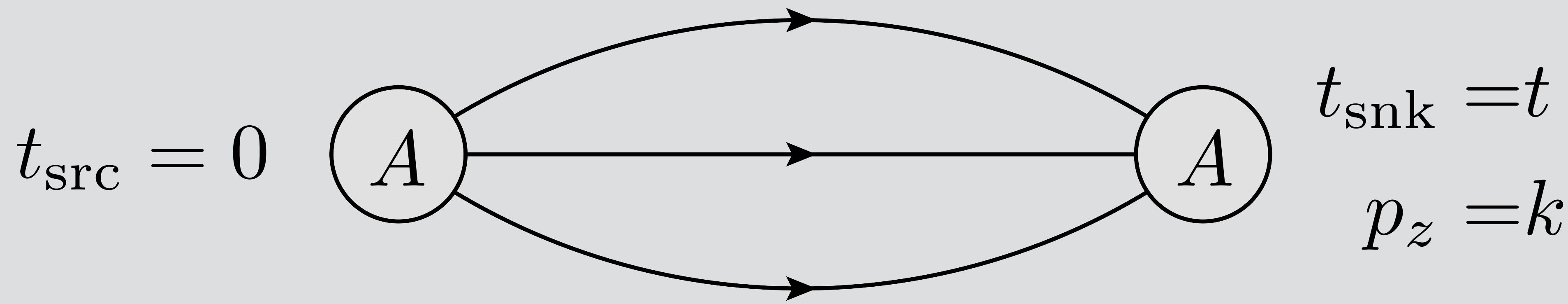
ETMC - position space method [1605.07327v1]

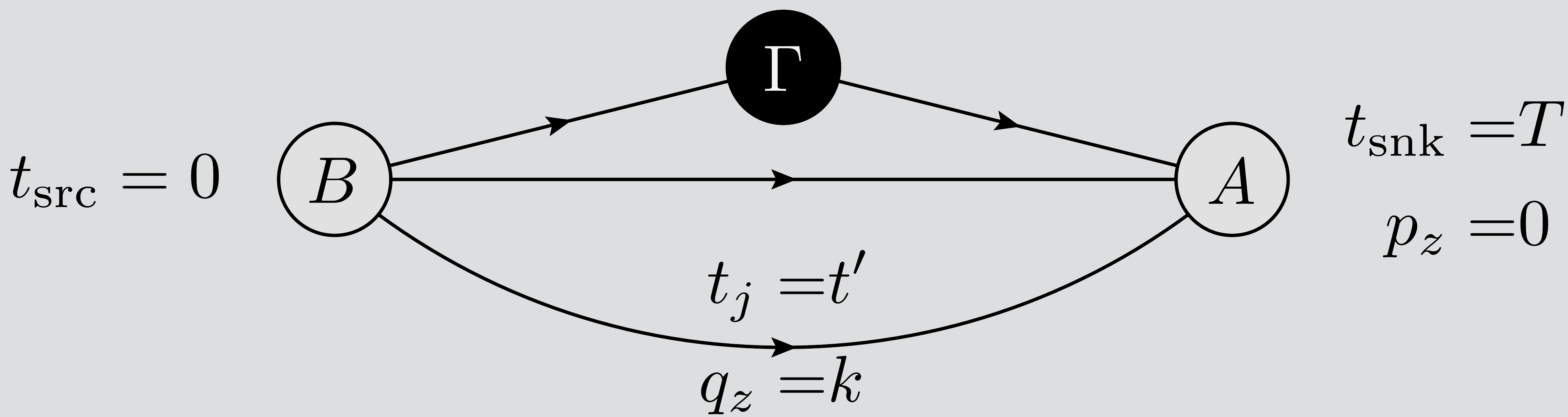
Most existing methods take $\partial/\partial q_j$ derivatives all at $q^2 = 0$

Our method takes $\partial/\partial q^2$ generalized to all momenta

Kinematic setup

Work done in collaboration with W&M JLab [1610.02354]





For charge radius $A = B = N^a$ the nucleon interp. operator

Two-point correlator and moment

two-point correlator

$$C_{2\text{pt}}(t) = \sum_{\vec{x}} \langle N^b_{t,\vec{x}} \overline{N}^b_{0,\vec{0}} \rangle e^{-ikx_z}$$

two-point moment

$$C'_{2\text{pt}}(t) = \sum_{\vec{x}} \frac{-x_z}{2k} \sin(kx_z) \langle N^b_{t,\vec{x}} \overline{N}^b_{0,\vec{0}} \rangle$$

$$\lim_{k^2 \to 0} C'_{2\text{pt}}(t) = \sum_{\vec{x}} \frac{-x_z^2}{2} \langle N^b_{t,\vec{x}} \overline{N}^b_{0,\vec{0}} \rangle$$

only have even spatial moments

Three-point correlator and moment

three-point correlator

$$C_{3\mathrm{pt}}(t,t') = \sum_{\vec{x},\vec{x}'} \langle N^a_{t,\vec{x}} \Gamma_{t',\vec{x}'} \overline{N}^b_{0,\vec{0}} \rangle e^{-ikx'_z}$$

three-point moment

$$C'_{3\mathrm{pt}}(t,t') = \sum_{\vec{x},\vec{x}'} \frac{-x'_z}{2k} \sin(kx'_z) \langle N^a_{t,\vec{x}} \Gamma_{t',\vec{x}'} \overline{N}^b_{0,\vec{0}} \rangle$$

$$\lim_{k^2\to 0} C'_{3\mathrm{pt}}(t,t') = \sum_{\vec{x},\vec{x}'} \frac{-x'^2_z}{2} \langle N^a_{t,\vec{x}} \Gamma_{t',\vec{x}'} \overline{N}^b_{0,\vec{0}} \rangle$$

moments are with respect to current insertion

given correlators, moments are computationally free

Spectral decomposition

two-point fit function

$$C_{2\text{pt}}(t) = \sum_m \frac{Z_m^{b\dagger}(k^2) Z_m^b(k^2)}{2E_m(k^2)} e^{-E_m(k^2)t}$$

two-point moment fit function

$$C'_{2\text{pt}}(t) = \sum_m C_m^{2\text{pt}}(t) \left(\frac{2Z_m^{b\prime}}{Z_m^b} - \frac{1}{2[E_m(k^2)]^2} - \frac{t}{2E_m(k^2)} \right)$$

definitions

$$Z_m^b(k^2) \equiv \langle m, p_i = (0,0,k) | \overline{N}^b | \Omega \rangle$$

$$E_m(k^2) = \sqrt{M_m^2 + k^2}$$

$Z_m^{b\prime} = 0$ for point source/sink

two-point constrains all parameters except $Z_m^{b\prime}$

More spectral decomposition

three-point fit function

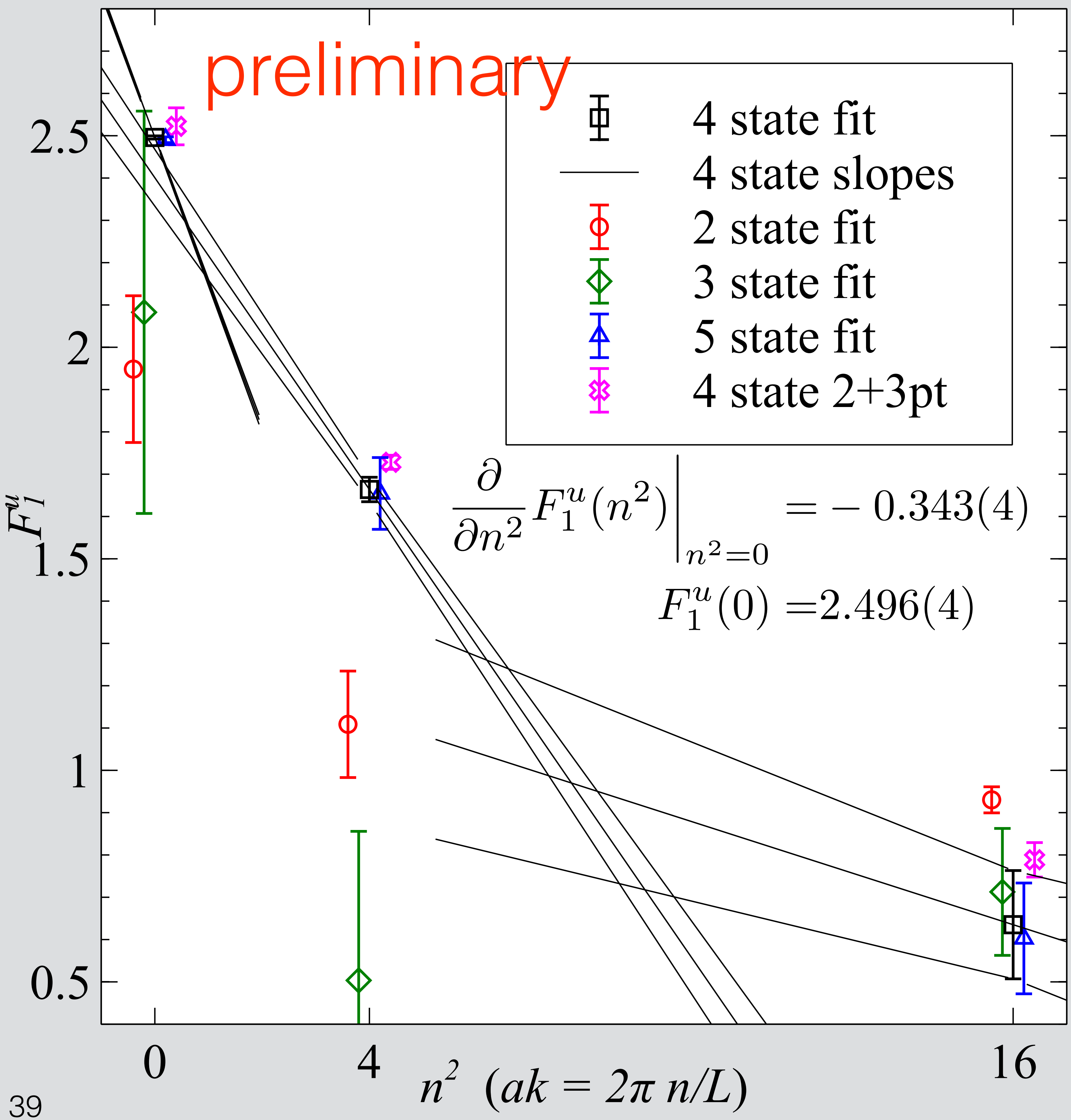
$$C_{3\text{pt}}(t,t') = \sum_{n,m} \frac{Z_n^{a\dagger}(0)\Gamma_{nm}(k^2)Z_m^b(k^2)}{4M_n E_m(k^2)} e^{-M_n(t-t')} e^{-E_m(k^2)t'}$$

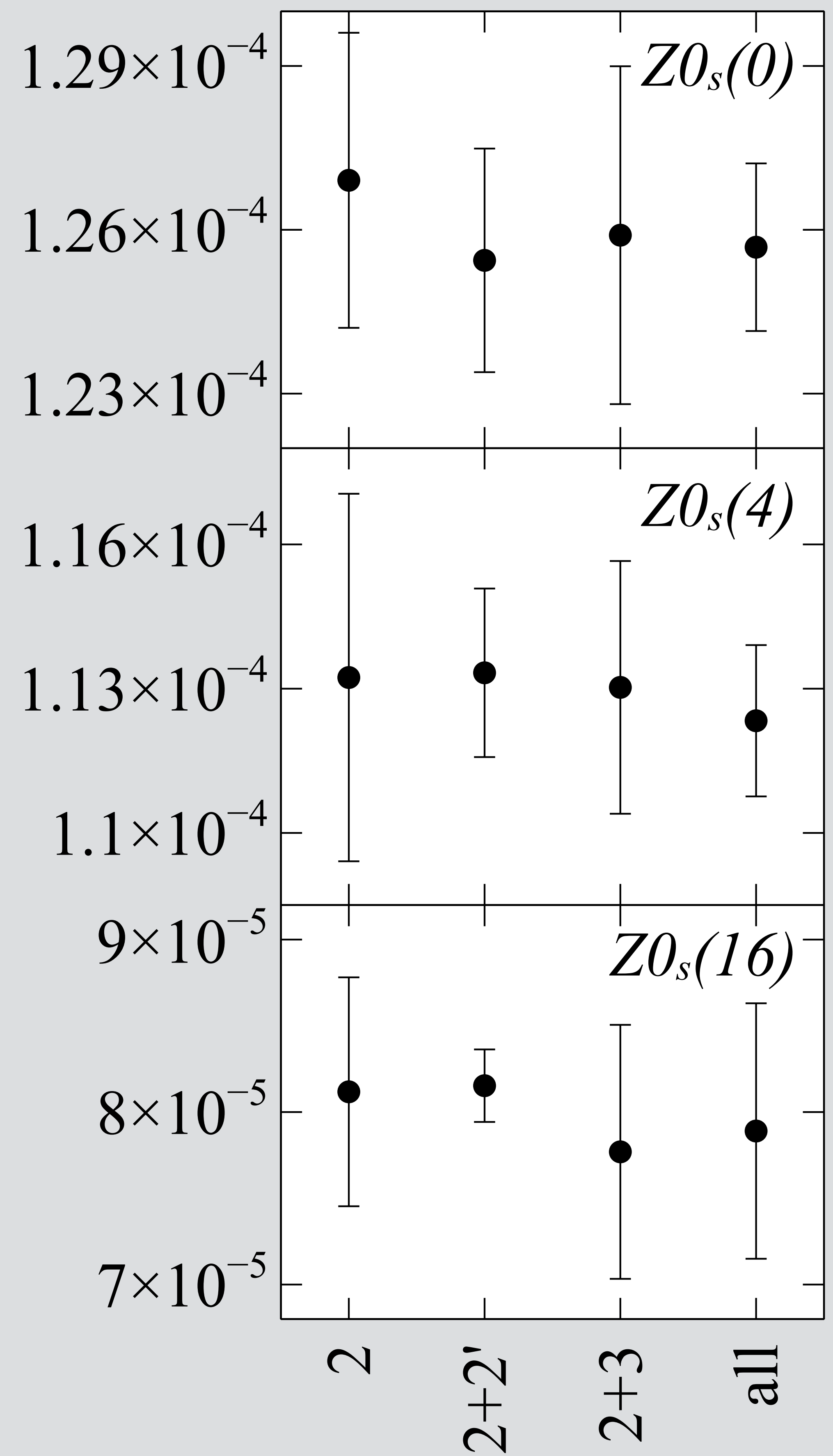
three-point moment fit function

$$C'_{3\text{pt}}(t,t') = \sum_{n,m} C_{nm}^{3\text{pt}}(t,t') \left\{ \frac{\Gamma'_{nm}}{\Gamma_{nm}} + \frac{Z_m^{b\prime}}{Z_m^b} - \frac{1}{2E_m^2} - \frac{t'}{2E_m} \right\}$$

2pt and 3pt constraints all params. except slopes
2pt moment needed for smeared source/sink
3pt moment constrains slope of form factor

Slope of nucleon vector form factor





Summary and Outlook

Lattice QCD is the only first principles method for studying spectroscopy and structure of hadrons

Hadronic matrix elements are essential for interpreting experimental results

Improved lattice calculation involves finding ever smarter ways to generate data (on top of hardware development)

Sophisticated analysis techniques are needed to extract the most out of very expensive data

Analysis and computing skills are very sexy in the Bay Area